Constraints on the Quasiparticle Density of States in High-T_c Superconductors

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In this Letter we present new tunneling data on $YBa_2Cu_3O_7$ thin films by low temperature scanning tunneling spectroscopy. Unusual peak-dip-hump features, previously reported in $Bi_2Sr_2CaCu_2O_{8+\delta}$, are also found in $YBa_2Cu_3O_7$. To analyse these common signatures we propose a new heuristic model in which, in addition to the d-wave symmetry, the gap function is energy dependent. A simple expression for the quasiparticle density of states is derived, giving an excellent agreement with the experiment. The dynamics of the quasiparticle states and the energy scales involved in the superconducting transition are discussed.

Getting to the heart of the quasiparticle density of states (DOS) in cuprate superconductors is an active goal of current theoretical and experimental research. Indeed, in the case of conventional materials, the quasiparticle DOS in the superconducting state contains the key information on the pairing. For this reason various methods, such as angle-resolved photoemission (ARPES), tunneling (TS) and Raman spectroscopies, as well as optical conductivity, are extensively used to elucidate the pairing mechanism in cuprates. Among these, scanning tunneling spectroscopy (STS), with its high spatial and energy resolution, emerges as the technique of choice.

Using such a local probe at low temperature, reproducible vacuum tunneling spectra have been obtained on many cuprates [1–8], in particular $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) and $YBa_2Cu_3O_7$ (YBCO). However, one still cannot interpret the experimental curves precisely. The shape of the DOS in BSCCO has a non-trivial dependence on doping [7,9,10], temperature [7,9–16] and magnetic field [17,18]. The state density is characterized by its large value at the Fermi level, unusual quasiparticle peaks and dip-hump structures at higher energies (see Fig.1). While the T_c vs doping curve is bell-shaped, the gap width decreases linearly, as the doping increases from underdoped to overdoped regimes, with no significant change in the DOS shape [7,9,10]. The temperature dependence is also unconventional: The gap does not vanish at the critical temperature and a pseudogap persists at $T > T_c$ [7,9,12–15]. Finally, a low temperature pseudogap remains when the superconducting order is destroyed, within the vortex core [18], or due to disorder [6]. All these features are difficult to explain with a BCS-type theory.

In this Letter we report our new low-temperature STS data on YBCO thin films. We observe strongly pronounced peak-dip-hump structures and a significant state density at zero bias. With previous data on BSCCO, our observations suggest a common mechanism for these features, linked to the superconducting state in cuprates. In order to clarify this effect, we propose a new quasiparticle DOS based on an energy-dependent gap function. A particular form for this function is inferred from the data and has, in addition to d-wave symmetry, a *single minimum* at a characteristic energy *near the gap value*. Using such a simple approach, all features (wide quasiparticle peaks, dips, humps and zero-bias) in the spectra of both YBCO and BSCCO may be properly fitted with remarkably few parameters. This procedure then allows one to follow the quasiparticle states dynamics in the phase transition, including the pseudogap. Moreover, the scaling of the dip position with the gap value at different dopings [7,9,10] is a natural consequence of the approach.

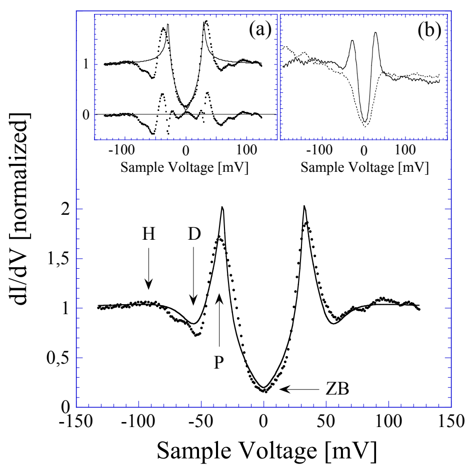

Fig. 1. dI/dV(V) spectra on BSCCO taken at $T = 4.2$ K (dots). The positions of the quasiparticle peak, dip, hump and zero bias, are indicated by P, D, H and ZB, respectively. Solid line: the fit by our heuristic DOS ($\Delta_0 = 46$ meV, $\delta_0 = 17$ meV, $A_0 = 0.45$, $\Gamma = 2.9$ meV).
Inset a: Experimental spectrum (dots) and d-wave fit (solid line) with an anisotropic normal Fermi surface as in [4]. Bottom curve: difference between experimental and d-wave fit.
Inset b: Superconducting DOS (solid line) and low temperature pseudogap (dotted line), measured in disordered BSCCO at $T = 4.2$ K.

It is now clear that, in a first approximation, the case of BSCCO is consistent with a d-wave gap function (inset (a) in Fig.1). However the dips and humps, observed

beyond the gap in the quasiparticle DOS (Fig.1), cannot be simply explained within this approximation. These features, existing at low temperatures, disappear at T_c [7,9,10], and thus should be related to the superconducting state. Using STS, Renner et al. [9] report on normal tip-superconductor (SIN) junctions, and find the dip to scale with the gap width for different doping levels, conserving its characteristic energy near -2Δ. This behaviour was confirmed in recent reports [7,10] where both superconductor-vacuum-superconductor (SIS) and SIN junctions with BSCCO were studied, and for a large range of carrier concentration. In the latter work, the dips were found at both negative and positive biases and at the energy near $\pm 3\Delta$ for symmetric SIS junctions and at $\pm 2\Delta$ for SIN ones. Similar behaviour was observed in ARPES measurements [11,12].

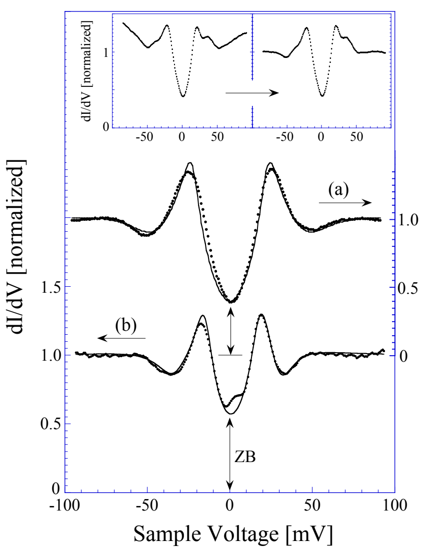

Fig. 2. Normalized tunneling spectra of YBCO at $T = 4.2$ K (dots). Solid lines: the fit by our new DOS function ($\Delta_0 = 37$ meV, $\delta_0 = 21$ meV, $A_0 = 0.5$, $\Gamma = 5.5$ meV for spectrum 1; $\Delta_0 = 26$ meV, $\delta_L = 14$ meV, $\delta_R = 11$ meV, $A_L = 0.7$, $A_R = 0.45$, $\Gamma = 8$ meV for spectrum 2).
Inset: Raw tunneling spectrum (left curve) observed in the same thin film of YBCO at $T = 4.2$ K. Right curve: The same spectrum, normalized to the parabolic background.

The quasiparticle DOS in YBCO was found to be different. Compared to BSCCO, a higher density of states at the Fermi level (30-60% zero-bias value), a significant parabolic background and double peaks, were observed [17]. However, no clear evidence for dip signatures were reported. We indeed observe spectra of this type in some locations of our thin films [19] (inset in Fig.2). However in most of the sample surface a second type of spectrum is found (Fig.2). The doubled peaks are absent there and a single broad peak is followed by strongly pronounced dips at both occupied and empty states. Another feature is an occasional anomaly at roughly +5 meV, similar to the resonant state observed in BSCCO and attributed to a point defect [20,21]. Comparing experimental curves, the shapes of our spectra in YBCO [22] and BSCCO are quite similar. These data clearly show that the large peaks, the dip-hump features and the important zero-bias background, are three signatures of the superconducting state in cuprates, and are not just a peculiarity of BSCCO [23]. None of these features are explained within a BCS-type weak coupling approach, even with some particular symmetry of the gap function. We now describe a new quasiparticle DOS, fitting in detail the tunneling spectra, and its consequences.

Consider a dispersion law of the general form: $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, where $\epsilon_{\mathbf{k}}$ is the normal state spectrum. In the case of a mean-field superconductor, the gap $\Delta_{\mathbf{k}}$ is either constant (strict BCS) or $\mathbf{k}$ dependent (BCS-type). In the latter case, of particular interest is the d-wave form: $\Delta(\varphi) \simeq \Delta_0 \cos(2\,\varphi)$, φ being the angle in the **a-b** momentum plane. Then, in polar coordinates, the superconducting tunneling DOS, $N_s(E)$, is written in terms of a spectral density $n_s(E,\varphi)$:

$$N_s(E) = \int_0^{2\pi} n_s(E,\varphi)\, d\varphi\ . \qquad (1)$$

Neglecting the angular dependence of the Fermi surface, the detailed conservation of states $n_n(\epsilon)\, d\epsilon = n_s(E,\varphi)\, dE$ leads to the expression:

$$n_s(E,\varphi) = n_n(E_F) \frac{E}{\sqrt{E^2 - \Delta(\varphi)^2}}, \qquad (2)$$

where $n_n(\epsilon) \approx n_n(E_F) = N_n(E_F)/2\pi$ is assumed for the normal DOS. Accounting for the anisotropy of the Fermi surface leads to the small correction: $n_n(E_F,\varphi)$ [4]. Finally, including some pair-breaking is equivalent to replacing $E \rightarrow E - i\Gamma$ and then taking the real part. As is well known, $n_s(E,\varphi)$ is singular at $E = \Delta(\varphi)$ and, when integrated over φ, gives the famous d-wave DOS widely used in the interpretation of the tunneling data. Having no other singularities, expressions of this general type cannot describe the experiment.

We go a step further by now assuming that the gap function depends on the quasiparticle states, while the dispersion law remains unchanged. A simple choice is of the form: $\Delta(\varphi) \rightarrow \Delta(E_k,\varphi)$, i.e. which ignores any *explicit* momentum dependence. The detailed conservation of the number of states follows analogously, giving a new expression for the superconducting spectral density:

$$n_s(E,\varphi) = \frac{1}{2\pi} N_n(E_F) \frac{E - \Delta(E,\varphi)\frac{\partial \Delta(E,\varphi)}{\partial E}}{\sqrt{E^2 - \Delta(E,\varphi)^2}}\ . \qquad (3)$$

Upon integration (1), the first term of the DOS is conventional, while the second term has a new and direct dependence on the gap function. This result should not be confused with strong-coupling, where the second term

in (3) is absent. In fact, this formula has been known for some time and was derived by J.R. Schrieffer [24]. It does not apply to conventional superconductors, in which retardation effects are crucial, and was therefore dropped.

We now focus on aspects of the spectra which determine the precise form of $\Delta(E,\varphi)$. Recent experimental [7,11,12] and theoretical [25] works have focused on the dip-hump features in BSCCO. However, we stress that the tunneling spectra of both BSCCO and YBCO are also characterized by unusually large quasiparticle peaks (much larger than the energy resolution of STS at $T = 4.2$ K) and an important zero-bias background, as in Figs.1 and 2. These aspects are even more striking if one plots the difference between the experimental data and the d-wave fit (inset (a) in Fig.1). The shape and magnitude of this difference curve lead to three straightforward conclusions. First, the difference curve is local: It is non-zero only within the energy range of a few Δ_0. Beyond these energies, there are clearly no important accidents in the curves. Second, a simple analysis of this curve shows that the number of states found above the d-wave fit is nearly equal to the number of states found below it, as the corresponding areas are compared. Thus, the effect is a strong but local modification of the mean-field quasiparticle DOS. Third, the general shape of the difference curve, in which a local maximum at one energy evolves into a local minimum at a higher energy, indicates that they both may arise from the derivative of a single peak at a characteristic energy situated somewhere between.

The above arguments, together with the fact that the peak-dip-hump appears at the critical temperature, at which the pair condensate is formed, indicate that the mechanism responsible for these features in the DOS should be reflected in the pair function: $\Delta(E,\varphi)$. Analytically, we choose a Lorentzian centered at $\pm|E_0|$ and with the characteristic width $2\delta_0$:

$$\Delta(E,\varphi) = \Delta_0 \cos(2\,\varphi)\,\left[1 - \frac{A_0\,{\delta_0}^2}{(E \pm E_0)^2 + {\delta_0}^2}\right]\;, \qquad (4)$$

where Δ_0 is the maximum value of the non-perturbed d-wave gap function and A_0 is the normalized amplitude (see inset in Fig.3). The use of (4) for $\Delta(E,\varphi)$ in (3) gives a new quasiparticle DOS having non-trivial characteristics (Fig. 3). This DOS has the usual 'd-wave' singularity, but at a new energy: Δ_{SC}, defined by $E = \Delta(E,0)$. In addition, two further extrema arise: a maximum rising near $E_0 - \delta_0$ and one minimum situated near $E_0 + \delta_0$, both being due to the derivative term.

At this stage the problem is already reduced to only five free parameters: Δ_0, E_0, δ_0, A_0 and the pair-breaking Γ. The fit to the experimental spectra with these parameters gives an excellent agreement. Surprisingly, the best fits do not situate Δ_0 at the quasiparticle peak but at some higher energy. Furthermore, the E_0 values are found to be nearly *equal* to Δ_0 for both BSCCO and YBCO spectra (solid lines in Fig.1 and Fig.2a respectively). For simplicity our calculated curves are taken to be symmetric with respect to zero energy, whereas the experimental spectra are clearly not. However, one can improve the quality of the fit considering δ_0 and A_0 to be different for the occupied and empty states in (4) (an example is given in Fig.2b).

In order to see how far the condition $E_0 \approx \Delta_0$ holds in general, we *a priori* set the resonance energy E_0 equal to Δ_0 in all other fits. In this way, with only four free parameters, we succeeded to fit almost all of our data. Consulting other reports [1–5,7], we find that our quasiparticle DOS should be widely applicable. The fits are not as good for the double peaked spectrum in YBCO, as in the inset in Fig.2. The expression (3) allows double singularities as shown in Fig.3d. However, they appear slightly smoother than in the TS curves. The possible reasons may be that the Lorentzian form (4) is too simple to reflect the orthorombicity of this cuprate, and its smaller anisotropy. These arguments seem plausible if one compares the tunneling data obtained in YBCO using STS [17] (double peaks) and those from planar junctions [26] (simple peaks). The role of structural or surface disorder cannot be excluded either, since in this work we observed the spectra of both types in the same thin film of YBCO.

The physical origin of the effect is thus a new coupling at the energy $E \simeq \Delta_0$ perturbing the quasiparticle spectrum in the superconducting state. In the non-superconducting state the interaction is either non-existant or inefficient and consequently $A_0 = 0$, and possibly $\delta_0 = 0$. The gap in the DOS is then $2\,\Delta \simeq 2\,\Delta_0$ (Fig.3a or Fig.3b). One may attribute this non-superconducting state to the pseudogap seen at low temperature [6,18]. Indeed, from the latter papers, where the pseudogap and superconducting gap were measured at the same temperature (4.2 K), one finds the pseudogap to be slightly larger than the superconducting gap (inset (b) in Fig.1). The values we find for Δ_0 are indeed larger than the peak-to-peak gap value Δ_{SC} extracted from the spectra. They are consistent with the low temperature pseudogap energy scale. The existence of two 'gap' scales (Δ_0 and Δ_{SC} in our approach) is also suggested in [27], where Andreev reflection experiments showed the gap of 28 meV, whereas the d-wave fit of the c-axis tunneling data gave 19 meV for the gap in the same system.

In the superconducting state the interaction term becomes non-zero ($A_0 > 0$) and two signatures appear in the DOS: An additional peak rises near $\Delta_0 - \delta_0$ and a dip near $\Delta_0 + \delta_0$. This dynamics comes from the derivative term in (3). Qualitatively the phenomenon corresponds to shifting states from $\Delta_0 + \delta_0$, to $\Delta_0 - \delta_0$ *inside* the gap Δ_0 (Fig.3, from (a) to (c) and from (b) to (d)). The main quasiparticle peak in the DOS results from the superposition of two peaks: one at Δ_{SC} and another at $\Delta_0 - \delta_0$, and explains why the quasiparticle peaks ap-

pear so large when they are not well separated (Fig.1 and Fig.2). In this Letter we do not discuss the state dynamics in the phase transition to the pseudogap state at $T = T_c$. This involves the explicit temperature dependence of the parameters $\Delta_0(T)$, $\Gamma(T)$ and $\delta_0(T)$, which are still controversial.

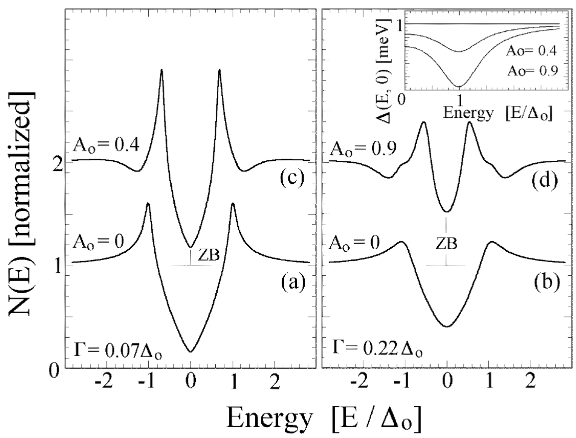

Fig. 3. Illustration of the state dynamics from non superconducting DOS, (a) and (b), to superconducting DOS, (c) and (d). In (c) Γ and A_0 are moderate: ZB is small, the peaks are single and well pronounced. In (d) Γ and A_0 are large: ZB is important, the peaks are broad and doubled, as reported in YBCO. For all curves $\Delta_0 = 37$ meV and $\delta_0 = 17$ meV. Inset: The shapes of the energy-dependent gap function used.

As is well known, in strong-coupling approaches to conventional superconductivity, the gap is energy dependent expressing the electron-phonon interaction. This perturbs the quasiparticle DOS at characteristic energies $\hbar\omega_{ph} \gg \Delta_0$ and is a second order effect. On the contrary, our gap function is modified significantly near Δ_0, leading to new singularities in the DOS to lowest order. In this sense they are an integral part of the superconductivity, the relevant parameters being the amplitude A_0 and the width $2\delta_0$ of the minimum in the gap function. The hump has no particular meaning in our model, being a consequence of the superposition of the dip with the slow decrease of the usual DOS tail.

In conclusion, we showed that the unusual peak-dip-hump features exist in both YBCO and BSCCO, being common peculiarities of the quasiparticle DOS in high-T_c cuprates. Experiments show that these signatures appear at $T \leq T_c$ and are intimately related to the superconducting phase. We suggest that the large peaks and dips observed in the superconducting state arise together from the same interaction, strongly perturbing the usual mean-field DOS. This unknown interaction is accounted for by introducing the energy-dependent gap function, having a minimum at E_0. The numerical analysis of the data showed that E_0 corresponds to the maximum value of the gap Δ_0 for all tunneling spectra in both BSCCO and YBCO. The natural consequence of this is the dip-hump scaling with the gap peak-to-peak value reported in [7,9]. Finally, the model suggests that the superconducting state differs from the 'normal' one by the non vanishing of $\partial\Delta/\partial E$. These results put strong constraints on a possible theory of the superconductivity.

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